OMNO2 README File

OMI NO_2 Algorithm Team

Document Version 6.2: July 31, 2012
Data Product Version 2.1

Species:	Nitrogen Dioxide (NO_2)
Data Version:	Standard Product, v2.1
Release Date of Current Version:	July 2012
Retrieved Quantities:	Total slant column density Total vertical column density Stratospheric column density Tropospheric column density
Spatial Resolution:	13 km x 24 km (at nadir)
Global Coverage:	Approximately daily
Date Range:	2004/10/01–Present
Data Screening:	See data quality flags in L2 data files
Data Location:	http://disc.sci.gsfc.nasa.gov/Aura/data-holdings/OMI
Primary Point of Contact:	Nickolay A. Krotkov NASA/Goddard Space Flight Center nickolay.a.krotkov@nasa.gov 301-614-5553

1. Executive summary

This README file describes the version 2.1 release of the OMI NO_2 Standard Product, OMNO2. The original, version 1 retrieval algorithm [*Bucsela et al*, 2006], was designed to infer as much information as possible about atmospheric NO_2 from the OMI measurements, with the minimum possible dependence on model simulations. This approach has continued with the development of the version 2.0 and 2.1 products.

OMNO2 version 2.0 represented a significant advance over version 1, and is in greatly improved agreement with independent NO_2 measurements [*Bucsela et al*., 2012]. During the five years since the version 1 release, research at NASA and other institutions has led to significant conceptual and technical improvements in the retrieval of NO_2 from space-based measurements, which have guided the development of the current version. In particular, the stratospheric estimate, based directly on OMI measurements, provides a more detailed and accurate stratospheric NO_2 field than did the wave-2 method of version 1. The tropospheric estimate has been improved using monthly, rather than annual, mean *a priori* NO_2 profiles, and by several improvements to the air mass factor calculations. Correction of calibration artifacts (destriping) has been improved, and identification and flagging of pixels affected by the OMI row anomaly has been added. We have also taken into account user suggestions regarding data format and ancillary information, which will make the NO_2 product more useful in research and applications. The overall structure of the data files has been simplified relative to version 1 for better usability, and we now provide scattering weight[*] profiles at each OMI pixel for averaging kernel calculations [see *Eskes and Boersma*, 2003]. Table 1 summarizes the changes. Version 2.1 makes incremental improvements to stratospheric estimates and destriping, resolves data gaps in high latitudes, improves the suite of metadata included with the Level 2 files, and removes a large number of deprecated fields.

Table 1. Summary of improvements in the version 2 Standard Product

Algorithm component		V1.0 Released 2006	V2.0 Released Fall 2011
Stripe correction		Based on data from 60S-60N of 15 orbits.	Based on data from 30S-5N of 5 orbits.
Stratosphere–troposphere separation		Stratospheric NO_2 field based on a global analysis that assumes a zonal wave-2 structure.	In regions of tropospheric pollution, stratospheric column is inferred using a local analysis of the stratospheric field.
Air Mass Factor (AMF)	NO_2 profile shape	GEOS-Chem annual mean tropospheric NO_2 profiles for the year 1997 coupled with a single stratospheric NO_2 profile.	Monthly mean NO_2 profile shapes derived from GSFC GMI CTM multiannual (2005-2007) simulation.
	Temperature profile	NMC monthly temperature profile climatology.	GEOS-5 monthly temperature profile climatology.
	Scattering weights (SW*)	SW table based on TOMRAD simulation.	Same, but with greater number of node points to reduce interpolation errors.
	Terrain albedo	GOME(-1)-based monthly climatology.	OMI-based monthly climatology.
	Tropopause pressure	Fixed tropopause pressure.	GEOS-5 monthly tropopause pressure.
	Cloud pressure/fraction	O_2-O_2 cloud algorithm.	Improved O_2-O_2 cloud algorithm.

[*] Also known as differential air mass factor (dAMF).

2. Introduction

Nitrogen oxides (NO_x = NO + NO_2) are species that play key roles in stratospheric and tropospheric ozone chemistry. Further, tropospheric NO_2 is recognized to be deleterious to human health. NO and NO_2 are in quasi-steady-state in the atmosphere, and their relative concentrations depend on temperature, solar illumination, and other chemical species. Major sources of tropospheric NO_x include combustion, soil emissions, and lightning. While NO is practically impossible to measure spectroscopically in remote sensing, NO_2 is readily measured. NO_2 column amounts are retrieved from measurements made by the Ozone Monitoring Instrument's (OMI) VIS detector in the spectral range 405–465 nm. The Level 2 (L2) NO_2 product (OMNO2) includes stratospheric, tropospheric, and total columns.

OMI was launched on July 15, 2004, on the EOS Aura satellite, which is in a sun-synchronous ascending polar orbit with a local equator crossing time (LECT) of ~13:45±0:05. Science-quality data operations began on October 1, 2004. OMI makes simultaneous measurements in a swath of width ~2600 km, divided into 60 fields of view (FOVs), or pixels. Fig. 1 shows the relative positions and sizes of these scenes transverse to the flight direction. One swath is measured every two seconds. Due to the optical characteristics of the instrument, adjacent swaths overlap considerably in ground coverage. The width of a swath ensures that swaths from adjacent consecutive orbits are nearly contiguous at the equator and have some overlap at mid- to high-latitudes. In a single orbit, OMI measures approximately 1650 swaths from terminator to terminator. With an orbital period of 99 minutes, OMI views the entire sunlit portion of the Earth in ~14.5 orbits.

For any position on the Earth, the OMI measurement time is generally not equal to the LECT. For near-nadir pixels, the local overpass time is generally earlier than the LECT in the Northern Hemisphere, and later in the Southern Hemisphere. Around latitudes 50 degrees, the difference, near-nadir, is about 1 hour, and can be much greater for off-nadir FOVs. In a swath the observational time is earlier for western pixels and later for eastern pixels (Fig.1). Appendix A describes how to calculate local times for OMI observations.

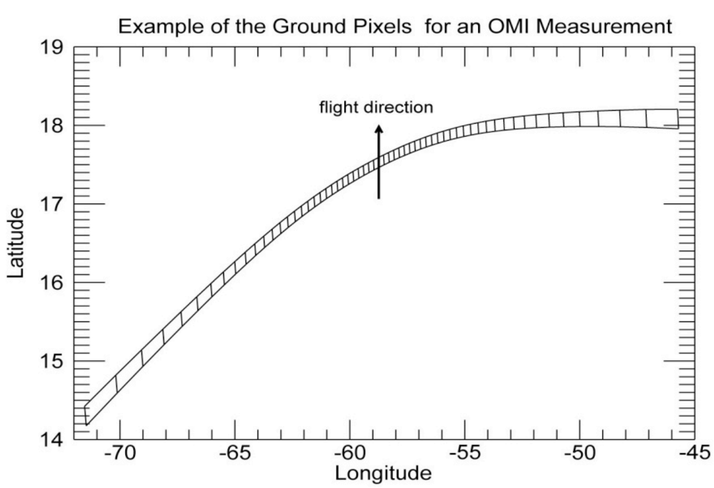

Figure 1. The position of 60 ground pixels for one OMI swath in the tropics. Due to optical aberrations and the asymmetric alignment between the instrument's optical axis and the spacecraft axes, the ground pixels are not symmetrically aligned with respect to the orbital plane. Note the different scales for the horizontal and vertical axes. The arrow shows the satellite trajectory.

Starting June 25, 2007, portions of the entrance optics appear to have been blocked, most likely by insulation material having debonded from the satellite body. Over time, the portion of the swath that is blocked has been changing. This phenomenon has been named the “row anomaly” (RA) referring to affected rows of the CCD detector. Detailed information may be found at http://www.knmi.nl/omi/research/product/rowanomaly-background.php. Although L2 OMNO2 values are calculated for all pixels, we recommend not using RA-affected pixels, as indicated by the XtrackQualityFlag field (see section 4).

3. File name

OMNO2 L2 files are written in HDF-EOS version 5 format and have the following naming convention [Aura guidelines, 2008; Claas 2011]:

```
<InstrumentID>_<DataType>_<DataID>_<Version>.<Suffix>,
```

where

```
<DataID> = <ObservationDateTime>-<Orbit#>
```

and

```
<Version> = <Collection#>-<ProductionDateTime>.
```

Below is an example of an OMNO2 L2 file name:

```
OMI-Aura_L2-OMNO2_2011m1010t2318-o38499_v003-2011m1011t154524.he5,
```

where:

<InstrumentID>	OMI-AURA
<DataType>	L2-OMNO2
<ObservationDateTime>	2011m1010t2318
<Orbit#>	o38499
<Collection#>	v003
<ProductionDateTime>	2011m1011t154524
<Suffix>	he5

4. Data description

As HDF-EOS5 files, OMNO2 L2 files contain a single swath, called ColumnAmountNO2, composed of a geolocation fields group and a data fields group. This section describes briefly the more significant data fields. A complete list of the fields and metadata information contained in the OMNO2 files can be found in the document: http://toms.gsfc.nasa.gov/omi/no2/OMNO2_data_product_specification.pdf

SlantColumnAmountNO2Destriped (*S*), and **SlantColumnAmountNO2Std:** are the retrieved slant column and its uncertainty. ***S*** is the retrieved total areal density of NO_2 molecules along the effective optical path from the sun into the atmosphere, and then toward the satellite. This is calculated from the measured Earthshine radiance and solar irradiance using the DOAS algorithm, with an NO_2 cross section measured at 220 K. Variations that are due to intercalibration of the detector cells have been removed using the destriping procedure described in section 5.

ColumnAmountNO2Strat and **ColumnAmountNO2StratStd:** Estimates of the stratospheric vertical column $\boldsymbol{V_{strat}}$, derived from S, and their uncertainty.

ColumnAmountNO2Trop and **ColumnAmountNO2TropStd:** Estimates of the tropospheric vertical column, $\boldsymbol{V_{trop}}$, derived from S, and their uncertainty.

ColumnAmountNO2 and **ColumnAmountNO2Std**: Estimates of the total (i.e., $\boldsymbol{V} = \boldsymbol{V_{strat}} + \boldsymbol{V_{trop}}$) vertical column and their uncertainty.

ScatteringWeight[†]**:** Vector **A** that describes the relationship between slant column, S_i and the vertical column, V_i, for each atmospheric layer *i*:

$$S = \sum_i S_i \approx \sum_i A_i \cdot V_i \tag{1}$$

A is relatively insensitive to the wavelength within the NO_2 spectral region, so only a single value, valid for the entire spectral fitting window, is provided. **A** is a function of the optical geometry, surface albedo, and cloud parameters, and contains a correction for the temperature dependence of the NO_2 cross section. SW is stored as a 3-dimensional array with dimensions [35, 60, 1644] (pressure levels, across track, along track[‡]). The grid of pressure levels is available in the file, as ScatteringWtPressure. The values, in hPa, are:

1020., 1010., 1000., 990., 975., 960., 945., 925., 900., 875., 850., 825., 800., 770., 740., 700., 660., 610., 560., 500., 450., 400., 350., 280., 200., 120., 60.0, 35.0, 20.0, 12.0, 8.0, 5.0, 3.0, 1.5, 0.8

Partial slant column (e.g. tropospheric) densities may be computed from Eq. (1) using ranges of *i* falling within the partial column, and V_i values derived from measurements or models. The partial column Air-Mass Factor (e.g. $\mathbf{AMF_{trop}}$, section 5.4) can be obtained by dividing Eq. (1) by the corresponding partial vertical column (e.g. $\mathbf{V_{trop}}$). Methods for comparing OMI columns with external datasets may be found in *Bucsela et al*. [2008], *Eskes and Boersma* [2003] and references therein.

XtrackQualityFlags: The cross-track quality flags indicate specific likely problems with the radiance measurements, due to the row anomaly (Section 2). As a general rule, for files with measurements after June 2007, one should not use data where the XtrackQualityFlags field is nonzero. However, before this time, the XtrackQualityFlags words are set to a fill value. Thus, the user should only use Level 2 data where

[†]SW is also known as box air mass factor (box-AMF) or differential air mass factor (dAMF).
[‡] The number of along-track positions varies from file to file.

XtrackQualityFlags is equal to zero, OR equal to the fill value. The fill value can be found in the field metadata; its value is FF_{16} (hexadecimal).

vcdQualityFlag: Quality assurance information for the tropospheric vertical column. The least significant bit is the summary quality flag. We recommend that most users only use data for which this bit is zero (i.e., vcdQualityFlag is an even integer).

5. Algorithm description

Figure 2 shows schematically the data flow through the algorithm. The individual steps are described in more detail in the following subsections.

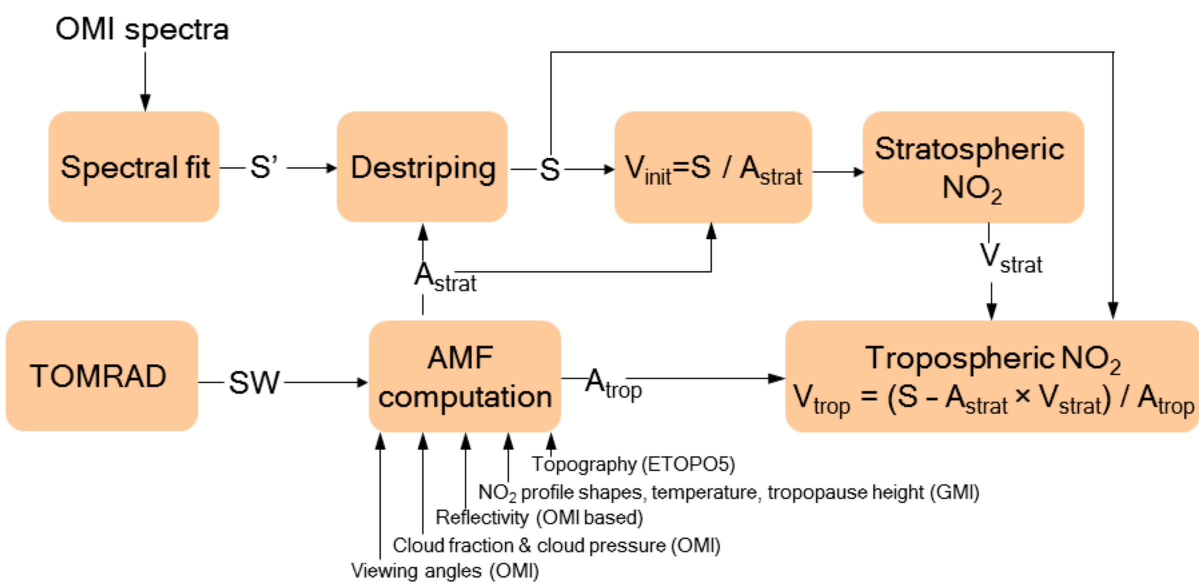

Figure 2. Schematic of the data flow through the OMI NO_2 algorithm. A_{strat} and A_{trop} are stratospheric and tropospheric Air Mass Factors (AMF) explained in section 5.2.

5.1 DOAS spectral fitting

The OMI Level 1b data product contains calibrated earthshine radiance spectra *I* for each pixel. Earthshine radiances are divided by a reference solar irradiance spectrum *F* to give a normalized spectrum *R* [$R(\lambda)=I(\lambda)/F(\lambda)$]. Use of a static solar reference spectrum ameliorated much of the calibration-induced striping that was discovered soon after OMI operations began. The normalized spectra are fitted to laboratory-measured trace gas spectra, a reference Ring spectrum [*Chance and Spurr*, 1997] and a polynomial function that models the spectrally slowly varying scattering by the atmosphere, clouds, and aerosols and reflection from the Earth's surface.

The fitting algorithm uses the Differential Optical Absorption Spectroscopy (DOAS) method, and is applied in the spectral range 405nm to 465nm. In the current version, the only trace gas absorption spectra considered are those of NO_2 [*Vandaele et al.,* 1998], O_3 [*Burrows, et al.*, 1999], and H_2O [Harder and Brault, 1997]. The trace gas absorption spectra used were produced by convolving high-resolution, laboratory-measured absorption spectra with the measured OMI slit function. The result of the spectral fit is a slant column density "SlantColumnAmountNO2" for each OMI pixel.

5.2 AMF calculation

The air mass factor (AMF) is defined as the ratio of the measured slant column *S* to the vertical column *V*. AMFs depend upon a number of parameters including optical geometry, surface albedo, and the shape of the NO_2 vertical profile. The **AMFs** are computed from the scattering weights (section 4) and a monthly mean climatology of NO_2 profile shapes constructed from the Global Modeling Initiative (GMI) Chemical Transport Model simulation. Stratospheric and tropospheric AMFs are calculated, ($\mathbf{A_{strat}}$ and $\mathbf{A_{trop}}$) separated by the climatological GEOS-5 monthly tropopause pressure. While stratospheric NO_2 retrieval is nearly insensitive to NO_2 profile shape assumption, tropospheric NO_2 retrieval is sensitive to the NO_2 profile shape and the temperature profile. Use of monthly NO_2 profile shapes captures the seasonal variation in NO_2 profiles [Lamsal et al., 2010]. The climatologies are available as ASCII files from Aura Validation Data Center (AVDC) site:
http://avdc.gsfc.nasa.gov/pub/tmp/OMNO2/OMNO2_reference_tables/

The method of AMF calculation is similar to that described by *Palmer et al.* [2001]. For each pixel, AMFs are computed for clear ($\mathbf{AMF_{clear}}$) and cloudy ($\mathbf{AMF_{cloud}}$) conditions. The AMF of a cloudy scene is calculated by:

$$AMF = (1 - fr) \cdot AMF_{Clear} + fr \cdot AMF_{Cloud} \quad (2)$$

where *fr* is the cloud radiance fraction (CRF), i.e. the fraction of the measured radiation that comes from clouds and aerosols. The CRF is computed from the effective cloud fraction f_c , using tables constructed from radiative transfer calculations, as part of the OMNO2 algorithm. Note that the CRF is usually larger than f_c, since the clouds are usually much brighter than the surrounding atmosphere at 440nm. $\mathbf{AMF_{clear}}$ is calculated assuming a Lambertian surface of reflectivity $\mathbf{R_s}$ at pressure $\mathbf{P_s}$. $\mathbf{AMF_{cloud}}$ is calculated assuming a Lambertian surface of reflectivity 0.8 at a pressure $\mathbf{P_c}$. $\mathbf{R_s}$ and $\mathbf{P_s}$ are obtained from a climatological database. $\mathbf{P_c}$ and f_c are obtained from the OMCLDO2 product. Please refer to OMCLDO2 readme file for relevant details.

5.3 Destriping

The measured NO_2 slant column densities are corrected for an instrumental artifact that varies across the orbital track and results in the appearance of “stripes” along the track. The severity of this artifact is greatly diminished by the use of a static solar spectrum (see section 5.1); however, further correction is needed. The destriping algorithm computes the mean cross-track biases using measurements obtained at latitudes between 30S and 5N and from orbits within 2 orbits of target orbit. These are essentially a set of 60 correction constants, one for each cross-track position, which are subtracted from the measured slant column densities to calculate the destriped slant column field, **SlantColumnAmountNO2Destriped** (see section 4). Although the uncorrected slant columns (**SlantColumnAmountNO2**) are also stored in the L2 files, we do not use them to calculate vertical columns.

5.4 Stratosphere–troposphere separation

The stratospheric and tropospheric column amounts are retrieved separately under the assumption that the two are largely independent. The stratospheric field is computed first, beginning with creation of a gridded global field $\mathbf{V_{init}} = \mathbf{S} / \mathbf{AMF_{strat}}$ values, assembled from data taken within 7 orbits of the target orbit. An *a priori* estimate of the tropospheric contribution to this field, based on a monthly GMI model climatology, is subtracted, and grid cells where this contribution exceeds 0.3×10^{15} cm^{-2} are masked. Masking ensures that the model contribution to the retrieval is minimal. Note that not all highly polluted areas will be masked in this procedure, since clouds may already hide the tropospheric NO_2 from OMI in those regions. A three-step (interpolation, filtering, and smoothing) algorithm is then applied to fill in the masked regions and data gaps, and to remove residual tropospheric contamination. The resulting stratospheric vertical column field, $\mathbf{V_{strat}}$, is converted to a slant column field using $\mathbf{AMF_{strat}}$, and subtracted from **S** to give the tropospheric slant column. Dividing this by the tropospheric air mass factor, $\mathbf{AMF_{trop}}$, gives the tropospheric vertical column $\mathbf{V_{trop}}$. For details see Bucsela et al., [2012].

6. Software versions

This document applies to the public release of the OMI L2 NO2 data, product version 2.1, archived as collection 3 and released in July 2012. The L2 algorithm is divided into four processes, each performed by a separate program. The end result is the creation of the OMNO2 L2 data product from the OMI Level 1b product. The software versions used to produce product version 2.1 are:

L0 to L1b processing	**collection 3**
OMCLDO2	**V1.2.3.3**
OMNO2A	**V1.2.3.1**
OMNO2B	**V1.2.1.0**
OMNO2	**V1.1.13.0**

7. Data Quality Assessment

The quality of the data in this release is currently being established by consistency checks and independent measurements in ongoing validation campaigns from ground-, aircraft-, and satellite-based instruments [Bucsela et al., 2012].

The fitting error in the NO_2 slant column is estimated to be 0.3–1x10^{15} cm^{-2}, before the row anomaly (RA). Users are advised against using RA affected data, indicated by a nonzero XTrackQualityFlag.

Preliminary comparisons of the retrieved stratospheric monthly zonal mean NO_2 columns show that they generally have increased slightly (<10%) relative to the version 1 retrieval. The seasonal variation of OMI stratospheric NO_2 agrees with the NASA GSFC GMI chemical transport model. An absolute bias of up to 25% exists, but is consistent with known model biases. A document detailing validation with other ground-based and satellite datasets is in preparation [Swartz et al., 2012].

The retrieved tropospheric NO_2 columns were compared with ground-based and in-situ NO_2 measurements and bottom-up emission inventories. The preliminary validation studies indicate a good agreement, considering several differences among the datasets. A detailed validation document is in preparation [Lamsal et al, 2012].

8. Product Availability

The OMNO2 product is archived and distributed from the Goddard Earth Sciences Data & Information Services center (GES DISC). The files can be directly downloaded from the GES DISC Mirador site which provides parameters and spatial subset capabilities. OMI products are written in HDF-EOS5 format. GES DISC also provides a list of tools that read HDF-EOS5 data files, see the link http://disc.sci.gsfc.nasa.gov/Aura/additional/tools.shtml.

9. Reporting Problems and Requesting Information

The following is a summary of links to current documentation for OMNO2:

http://toms.gsfc.nasa.gov/omi/no2/OMNO2_readme.pdf
http://toms.gsfc.nasa.gov/omi/no2/OMNO2_data_product_specification.pdf

To report problems, or pose questions and comments related to the OMNO2 algorithm, data quality, and file structure, please sends electronic mail to the OMI NO_2 algorithm team: omno2@ltpmail.gsfc.nasa.gov. Additional questions may be directed to the principal point of contact for OMNO2: Nickolay.A.Krotkov@nasa.gov

10. References

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Appendix A: Time Calculations

The local mean, civil, or apparent time at the center of any OMI pixel can be obtained from the geolocation data, using the variable "Time" for the swath and the variable "Longitude" for the pixel. (Apparent time requires, additionally, calculation of the Equation of Time.) The Time variable is given in decimal TAI-93 format, so should be converted (for sub-minute precision) to UTC. The local solar times—mean and apparent—are of importance when the photochemical lifetimes of NO_2 are important. The relevant equations are:

UTC	= TAI – 32 – LS	(Coordinated Universal Time)
LCT	= UTC + TZ	(Local Civil Time = Wall-clock time)
LMST	= UTC + λ/15	(Local Mean Solar Time)
LAST	= LMST + E	(Local Apparent Solar Time = Sundial time)

Where

LS	= Number of leap seconds added since July 1, 2004 (One-second additions occurred at midnight after Dec. 31, 2005, Dec 31, 2008, and June 31, 2012)
TZ	= Time zone value (e.g. −4 hours for US Eastern Daylight Time)
λ	= Longitude, in degrees (East positive, West negative)
E	= Equation of Time.

The Equation of Time, in minutes, can be approximated with a precision of < 6 s by the formula

$$E = 9.87 \sin(2B) - 7.53 \cos(B) - 1.5 \sin(B)$$

where

B	= 360 (DOY – 81) / 365.
DOY	= Day of Year

Formulae for higher-precision calculations of E can be found in various reference sources.